Optics at the Advanced Photon Source: Strategic Needs and Plans

X-ray Science Division, Optics Group

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The purpose of this Optics Strategic Plan is to describe the Advanced Photon Source (APS) Optics Group's strategies for the next five years to develop state-of-the-art optics to support the missions of the APS and the U.S. Department of Energy (DOE) Office of Basic Energy Sciences (BES).

The first version of this plan was prepared during March 2015 as part of the documents and material submitted to the APS Optics Advisory Committee for review during its first meeting on March 15, 2015.

The present revision describes the status of the Optics Group's activities and updates our short- and long-term plans up to the year 2020.

1. Background and APS Optics Group mission

The forefront basic and applied research that is the mission of the APS relies heavily on beamline and end-station optics for x-ray energy, bandwidth, and polarization selection, as well as coherence preservation, collimation, and focusing. APS beamlines require high-quality x-ray optics (such as monochromators, mirrors, and focusing optics) to deliver an x-ray beam to the sample, and in many cases to collect the relevant signal from the experiment (such as by using crystal analyzers). As we prepare for a proposed multi-bend achromat (MBA) lattice to upgrade the APS, we must optimize the APS beamline optics by developing new optics or improving existing optics to fully exploit the new source parameters that will lead to a much smaller radiation source, larger spatial coherence, and more than a 100-fold increase in brightness. The majority of existing APS beamlines still utilize optics that date back to the construction of the facility roughly two decades ago. Optics fabrication technologies have improved considerably since then, and new focusing optics approaches have been developed, so there is considerable room for performance enhancements even with today's source parameters.

As noted in the 2013 DOE workshop report, "X-ray Optics for BES Light Source Facilities," the development of ever more powerful x-ray sources in the near future requires a new generation of x-ray optics that will allow us to fully utilize these beams. Consequently, as part of achieving readiness for the APS Upgrade (APS-U), the performance of X-ray Science Division (XSD) beamlines is being evaluated by measuring key parameters including flux, beam size, vibration and coherence. The data collected, together with beamline simulations, will be used for future optimization and improvement. To date, 14 beamlines (serving 20 endstations) have been evaluated. The majority appear to be operating with non-ideal optics and environmental conditions. The measurements showed that the performance of most beamlines is affected not only by the quality of the optics, but also by vibration and instability of the opto-mechanics. Therefore, our strategy is to take into account the performance of the entire optics assemblies in the design, implementation, and integration of beamline optics in coordination with the APS beamline scientists and resident users, and support group within the XSD and APS engineering groups.

The Group's activities and its R&D goals for 2016 and beyond are focused on the following key areas, which are discussed in this Strategic Plan:

- Develop advanced beamline optics modeling, simulation, and optimization tools;
- Develop advanced crystal monochromators for wavefront preservation, high-heat-load applications, and high energy resolution;
- Develop new mirrors in collaboration with industry, and refurbish existing mirrors using a new in-house deposition system;
- Develop advanced thin-film optics, including single-layer and multilayer optics;
- Develop micro- and nanofocusing optics, including high-aspect-ratio Fresnel zone plates, profile-coated Kirkpatrick-Baez (K-B) mirrors, and multilayer Laue lens (MLL) optics;
- Develop new cooling technologies for monochromators for high-heat-load applications;
- Develop coherence-preserving mirrors in collaboration with industry and other DOE light sources;
- Develop adaptive x-ray mirror systems in collaboration with other light sources and industry; and
- Develop advanced characterization tools and carry out optics characterization on all of the above.

We present here the Optics Group's R&D capabilities and strategies for meeting both present APS operational needs and the needs of the APS-U. One part of our strategy involves working directly with vendors to acquire and characterize the desired optics, such as beamline mirrors, standard monochromators, and other commercially available optics such as standard compound refractive lenses (CRLs) and capillary optics. The other part involves the use of in-house capabilities to develop one-of-a-kind optics that cannot be acquired from a vendor. To this end, the Optics Group has a wide range of fabrication and optical and at-wavelength characterization tools. We also work closely with the other DOE/BES light sources as well as with other research institutions and industry to leverage the APS state-of-the-art optics facilities and capabilities.

2. Beamline optics simulation and optimization

2.1. Status

Optics development begins with design and simulation, and this area has been significantly strengthened within the past two and a half years by strategic staff hiring in the Optics Group. Though existing codes based on ray tracing (e.g., SHADOW) and wavefront propagation (e.g., SRW) have been widely used in the past, improvements and new developments were needed. These have already begun to emerge as part of a new code which uses a hybrid approach combining ray tracing and wavefront propagation. The former addresses the geometrical aspects of the optics and the latter takes into account the diffraction when apertures clip the beam. The main advantage of the Hybrid code, developed in collaboration with the European Synchrotron Radiation Facility, is its speed compared to existing codes. This code is ray-tracing-based and includes diffraction effects from apertures and beamline optics by means of wavefront propagation. It is able to deal with partial coherence and figure errors in optics and is already serving as a crucial guide for the design of beamline optics required for the APS-U.

2.2. Strategic plan

By the end of FY 2016, optics simulations will be performed to support the preliminary design of new APS-U beamlines. The Hybrid code will be enhanced by including fast two-dimensional simulations, better undulator source models, and other optics implementations such as CRLs.

By the end of FY 2017, all APS beamlines will be simulated to prepare for the APS-U. Data analysis software for optics characterization will be developed for coherence measurement and wavefront sensing. A simulation package that combines heat load calculation and ray tracing will also be developed. Future R&D within the next five years will include developing packages for propagating Wigner functions or cross-spectral density functions through beamline optics. The above work will be carried out in coordination with other DOE light sources as well as with other synchrotron radiation facilities worldwide.

3. Crystal optics

3.1. Status

Nearly every beamline at the APS uses one or more crystal-based x-ray optics. Supporting APS as the nation's premier hard x-ray facility, crystal optics play a crucial role at the APS in x-ray monochromatization (including under high heat load) and in high-resolution spectrometers and analyzers. The Optics Group has considerable expertise in both designing and modeling crystal optics systems and in fabricating crystal optics throughout the entire pathway from silicon boule machining to crystal orienting and cutting with ~0.1° accuracy, super-smooth and strain-free crystal polishing (with RMS roughness ≤2Å), and x-ray topographic characterization. The Group's operational efficiencies are enormous, in that every year the team delivers hundreds of standard or highly customized monochromators, analyzers, beam splitters, polarizers, etc., to both the APS beamlines and other DOE/BES light source and neutron facilities.

Ongoing R&D efforts include the development of efficient sub-10-meV (as well as sub-1-meV) analyzer systems; bent-crystal monochromators for high efficiency at up to 100 keV; crystal optics based on exotic materials such as sapphire, quartz, and, in particular, diamond for high-heat-load beam splitting; optics for x-ray free electron laser oscillator cavities; and other applications such as diamond crystal optics for FEL self-seeding, which includes research efforts by APS staff beyond the Optics Group.

3.2. Strategic plan

Availability of wavefront preserving crystal optics is essential for imaging beamlines as well as for those requiring high resolution and diffraction limited focusing. To meet the APS MBA needs in area, the Optics Group R&D activities focus on the following:

- Development of crystal orienting capability to <0.01 deg.;
- Development of capabilities for strain-free polishing of crystals to achieve ≤1-Å rms surface roughness; and
- Development of etching and polishing procedures to fabricate strain-free crystal monochromators and analyzers using new materials beyond silicon, such as germanium, diamond, quartz, sapphire, and lithium niobate.
- Improvements in channel cut crystal polishing
- Simulation and coherence characterization

Significant progress can be made at the APS in these area because: (a) crystal fabrication and polishing available in the Optics Group is unique in the US, (b) grating interferometry has been developed and used for measurements of spatial coherence lengths at beamline 1-BM at the APS; and (c) an optics test beamline, 1-BM, is now available and can be used to explore theoretical predictions.

4. Beamline mirrors

4.1 Status

Large grazing-incidence mirrors are essential components of the APS, and are usually delivered by commercial vendors. Many APS beamline mirrors were installed as far back as 20 years ago, when the best mirrors of this type had slope errors of ~5,000 nrad and surface roughness of ~0.5 nm rms. Simulations show that the APS MBA lattice upgrade will require mirrors with slope error better than 150 nrad rms over 1 m in length, and roughness ≤0.1 nm rms. A state-of-the-art flat silicon mirror could cost as much as $50K to $100K, not including the support and mounting system, and would require at least 6 to 10 months' lead time for fabrication, depending on the manufacturer.

4.2 Strategic plan

It is conceivable that most of the existing APS mirrors could be improved by stripping off their coatings and deterministically figure-correcting their surfaces (as demonstrated at Diamond Light Source in the UK) so that they meet the future APS MBA lattice source's requirements, thus saving significant cost and time. Therefore, our strategy for mirrors includes two components: 1) refurbish as many existing mirrors as possible using the Modular Deposition System (MDS) described below; and 2) for special mirrors and new mirrors, work closely with vendors to develop procedures that will enable them to fabricate mirrors with the required surface specifications. This collaborative work will be done through simulation and modeling, with validation by optical metrology and at-wavelength metrology and characterization at bending-magnet beamline 1-BM or an insertion device beamline as required.

5. Thin-film optics

5.1. Status

Originally, the thin-film facility at the APS was intended for coating of single-layer films on large substrates to produce simple x-ray mirrors. As the field progressed, new equipment and new expertise were added in order to produce simple multilayer mirrors for user applications. With science needs driving the x-ray optics, and x-ray optics enabling new scientific capabilities, it has become clear that the APS must invest in thin-film infrastructure in order to meet mission needs both at the present time and in the era of the future APS. As a result, a new vacuum-processing instrument, the MDS, has been designed by the APS, procured during FY 2015, and delivered in February 2016. The system includes thin-film deposition, ion milling for figure correction, and *in situ* surface figure metrology. The equipment consists of a large, linear substrate translator housed inside a vacuum chamber. This substrate translator incorporates a state-of-the-art, direct-drive, in-vacuum servo system. The machine incorporates large, vertically planar cathodes, ion beam milling, and *in situ* metrology required for future APS MBA lattice upgrade mission needs. The system has accommodations to allow for mirror figure modification or correction with a combination of ion beam milling, profile coating, and *in situ* metrology.

5.2. Strategic plan

R&D on figure correction and *in situ* metrology is currently under way with strategic Laboratory Directed Research and Development funding. Provisions for a dynamically actuated aperture will be used to explore methods for three-dimensional multilayer deposition intended to enable the use of new optical geometries and to allow for higher efficiency and mirror figure correction. Such new optics will enable frontier science, utilizing new methods of inelastic x-ray scattering and small angle x-ray scattering. This area was explicitly called out in the 2013 DOE x-ray optics workshop report as one of the Grand Challenges. In fact, the new MDS can be put to use in exploring three of these Grand Challenges and providing experimental verification for the fourth.

6. Nanofocusing optics

Pushing x-ray microscopy into the nanoscale is crucial for understanding complex hierarchical devices on length scales approaching the atomic dimension. Nanoprobe experiments (including coherent-diffraction variants such as ptychography) require a high degree of spatial coherence to achieve a focus limited by diffraction from the optics. The 100-fold brightness improvement expected from the APS-U translates directly into increased coherent flux for these experiments. This transformative change allows one to achieve higher spatial resolution, scan larger areas, and image more representative sets of specimens. There are still beamlines that either lack adequate focusing optics or are in need of further optimization to take full advantage of the APS properties. Furthermore, the planned APS MBA lattice upgrade is expected to deliver beams with a much smaller emittance and a 100- to 1000-fold increase in coherent flux at high x-ray energies in the multi-ten-keV range compared to the current APS, thus underscoring the need to further pursue the development of high-energy x-ray focusing optics. R&D in this area includes focusing capabilities of multilayer optics, MLLs, and total reflection mirrors, improvement of refractive optics such as sawtooth lenses and CRLs for sub-micron focusing, bent crystal optics for focusing, etc. Our three primary areas of strategic development in nanofocusing optics are discussed below.

6.1. Fresnel zone plates: status

Fresnel zone plates remain the optics of choice for many x-ray microscopes because of their compactness, simple normal-incidence alignment, and large imaging field. Traditionally, they have required compromises on either resolution (determined by the narrowest fabricated zone width) or efficiency (determined by the thickness of the zone material) because of limitations on achievable nanofabrication aspect ratios. However, recent developments have widened the horizon for Fresnel zone plates for hard x-ray nanofocusing by improving high-aspect-ratio nanofabrication methods and intermediate-field zone plate stacking. In alignment with the APS-U and future operations needs, the primary goal for the next few years of Fresnel zone plate development is 20-nm focusing at 25-keV x-ray energy and 20% focusing efficiency.

Drawing upon Argonne National Laboratory's strengths in nanolithography and atomic layer deposition, a team effort has begun on developing zone plates using both direct photoresist writes and gold electroplating, and the zone-doubling process developed at the Paul Scherrer Institute. The collaborative effort has resulted in a demonstration with multiple zone plate layers written on a single substrate and 60:1 aspect ratios using the metal-assisted chemical etching process that has been utilized in recent zone plate fabrication experiments at SLAC. For high-efficiency focusing at high energy, zone plates will be stacked in the near and intermediate field to achieve the desired zone thickness. It has long been known that multiple zone plates can be stacked together in the near field to enhance hard x-ray focusing efficiency. More recently, it was shown that one can stack multiple zone plates at farther, more practical distances from each other, provided that each zone plate design is tailored for its position. A cross-divisional team from the Optics, Microscopy, and Imaging groups in XSD, and the APS Engineering Support Division, has demonstrated the stacking of six zone plates to achieve 28% efficiency at 27 keV.

6.2. Fresnel zone plates: strategic plan

Development of both near-and far-field stacking techniques will proceed in parallel with zone plate fabrication development to try to improve the focus spot size and efficiency simultaneously. Taken together, these new developments in high-aspect-ratio zone plate fabrication and zone plate stacking promise high-resolution, high-efficiency nanofocusing. By the end of 2016, the fabrication process for zone plates with 20:1-aspect-ratio zones down to 16 nm in width will be developed to meet the APS-U goal. Also, sets of zone plates with 40- and20-nm zone widths will be stacked to test the stacking-apparatus capabilities at these fine zone widths to guide engineering improvements. The Optics Group will continue to improve the capabilities at APS beamlines by incorporating the zone plates that are developed.

6.3 Kirkpatrick-Baez mirrors: status

Mirrors used for nanofocusing can provide higher efficiency than diffractive optics if the same numerical aperture is used, and they can be achromatic for spectroscopy if one uses simple specular reflectivity. Two-dimensional focusing with a K-B mirror pair can be accomplished either by bending a properly shaped flat optic into an elliptical form, or by pre-figuring a mirror with a fixed elliptical surface (the latter approach is used for stable nanofocusing applications). The APS has a long history of producing profile-coated mirrors for submicron- and nanofocusing applications. These mirrors are fabricated by depositing a profiled platinum thin film through a figured mask on either a flat or a spherical substrate to generate an elliptical shape. This method provides a quick and cost-effective way to produce fixed-geometry K-B mirrors to match custom beamline configurations at the APS.

A new profile-coating system for mirrors less than 150 mm long has been commissioned at the APS, replacing a system with lower performance. This new deposition system has already been used to fabricate K-B mirrors for sub-micrometer focusing. The best prototype profile-coated K-

B mirrors produced so far at the APS have a focus of approximately 75–85 nm, and 200-nm to 1-µm focus for routine use. The Optics Group worked with the APS Engineering Support Division to incorporate these into an in-house-designed mounting system and then pre-aligned and characterized the full mirror assembly at beamline 1-BM prior to delivery for experiments at 8-BM. This integrated system approach marks a significant advance over past practices, where profile-coated mirrors were delivered to APS beamline scientists as single components.

6.4 Kirkpatrick-Baez mirrors: strategic plan

At present, the main limiting factors in profile-coated K-B mirror technology are metrology and the deposition system. *In situ* metrology will be incorporated in the new MDS for *in situ* monitoring of mirrors during ion milling and profile coating, but an *ex situ* metrology tool will be required both to use as a backup system and to evaluate future advanced beamline mirrors procured from vendors. The new MDS will enable the exploration of new coating materials, which might have better long-term stability than the metal coatings now used for in-air mirror systems.

6.5 Multilayer Laue lenses: status

MLLs offer a path toward sub-10-nm focusing, especially for fixed-energy experiments. While these optics were conceived and first demonstrated at the APS, the National Synchrotron Light Source II project at BNL has chosen to concentrate on their development. Focusing below 15 nm in the hard x-ray regime has already been demonstrated, and an MLL that doubled the largest aperture ever achieved to 102 microns was measured to have efficiencies of more than 13% at 12 keV at beamline 1-BM. However, much R&D effort is required to produce sub-5-nm focusing and functional optics for day-to-day operation. This effort includes research on new bi-layer material combinations to increase efficiency, optimum deposition parameters and conditions to reduce built-in stress, etc.

6.6 Multilayer Laue lenses: strategic plan

The new APS MDS will have capabilities complementary to those at BNL for MLL development (such as better control of partial gas pressures for thick-film stress control and 1-ampere substrate biasing capability), enabling the APS Optics Group to continue to contribute to MLL R&D in collaboration with BNL.

7. High heat load and thermo-mechanical stability

7.1 Status

Liquid-nitrogen-cooled silicon has remained the monochromator cooling method/material of choice at the APS since the facility's commissioning in the early 1990s, and is expected to remain so for the APS-U. The reason is because the thermal expansion coefficient become at about ~124 K and the thermal conductivity improve by about an order of magnitude compared to room temperature. Many different cooling schemes are being used or tried, including internal cooling channels, side cooling, and hockey-puck geometry. Because of their ease of maintenance, water-cooled diamond monochromators are also used, particularly in beamlines where the narrower bandwidth of diamond compared to silicon is either desired or not an issue. Since the APS began its operations, much has been learned about silicon monochromator cooling efficiency and mounting stability and design. Side cooling has proven to be the most effective approach for mitigating heat load on silicon monochromators.

7.2 Strategic plan

The APS MBA upgrade will likely increase the power load on the first beamline optics. While the power density increase for single undulator will be less than a factor of two, and, therefore, a standard liquid nitrogen cooled monochromator could work, much R&D will be required to meet the needs of the most extreme cases, such as when two undulators are used in series. More specifically, realizing the full potential of the APS MBA source may require high heat load monochromator assemblies that provide minimal thermo-mechanical distortions along with outstanding opto-mechanical stability. Simulation studies and testing may be required to determine the optimum cooling geometries needed to minimize the impact of thermal distortions on the transmitted wavefront; that is, to preserve brilliance and to do so while maintaining angular stability at better than 50 nrad.

Indirect cooling of high-heat-load monochromators is highly advantageous compared to direct cooling because of its simple design, reduced maintenance, and low flow-induced vibration. However, it is generally achieved through an indium foil clamped between the optics surface to be cooled and a copper cooling manifold. As a result, the cooling efficiency depends heavily on the conformance of the interface material (i.e., the indium foil) and the clamping force. We plan to investigate a new approach which based on nano-bonding of the cooling manifold to a crystal monochromator. Preliminary tests conducted at the APS showed encouraging results. We intend to study a variety of bonding materials and cooling geometries and evaluate their effect on the silicon crystal lattice strain and the cooling efficiency.

If successful, this approach could pave the way to developing a set of standard APS monochromator designs that beamlines can adopt with assurance that they will handle the power load of the APS-U, preserve source brilliance, and offer improved stability. The technology could be equally applied to mirrors and multilayer optics.

8. Coherence-preserving mirrors and windows

8.1 Status

The MBA lattice upgrade of the APS will deliver x-ray beams with a much higher degree of coherence, and those coherence properties must be preserved as much as possible while the beam is manipulated using x-ray optics. The current and future capabilities at the APS for producing nanofocusing mirrors with profiled deposition, or correcting figure errors with a combination of *in situ* metrology and either ion-beam figuring or differential deposition, are directly applicable to exploration of coherence-preserving mirrors, since many of the surface finish and figure requirements are similar.

Finite element studies showed that, under the APS MBA beams, if used as the first beamline optics, water cooled mirrors will be significantly distorted. This in turn will dramatically alter the source and beam wavefront properties. With two undulators in series, the power load will double, which renders water cooling totally inefficient. Here, to preserve the source brilliance, liquid nitrogen cooling may be necessary.

Beryllium windows have been reported to act as an additional effective source, with the consequence that a portion of the radiation has a sharply reduced coherence length after passing through a window far downstream of an undulator. The net effect was reported to produce a sharp intensity peak in the center of coherent diffraction images of nanocrystals. Other deleterious exit-window effects have been found in topographic studies. A sizable body of work has been done at SPring-8 (Japan) on both beryllium and diamond windows, including characterization using shearing interferometry. PETRA III (Germany) has also employed diamond exit windows.

8.2 Strategic plan

Diamond as an optical element—for use as windows, substrates for fabrication of x-ray optics, reflecting surfaces, or otherwise—will continue to have an increasing impact on light source facilities worldwide. The Optics Group will continue to monitor the current status of polycrystalline and single-crystal diamond growth and fabrication techniques in order to best serve the APS community.

A supply of acceptable mirrors, window materials and multilayer substrates will be ensured through close collaboration with vendors. Samples produced by different vendors will be studied to select optimum window materials and mirror and multilayer-substrate polishing methods. Related coherence measurement and beam wavefront characterization work will be performed at beamline 1-BM or, if necessary, at an insertion device beamline. This work will be conducted by a postdoctoral appointee to be hired during 2016. R&D and testing must be conducted on cryo-cooled mirror and determine a cooling geometry that best preserve the beam integrity. This effort will be supported by the APS-U.

9. Adaptive and beam-shaping optics

9.1 Status

Even the best reflective optics available today have some residual slope and form errors, which affect their nanofocusing properties, and some scientific applications are best served by mirrors that have variable focal lengths or produce designed beam profiles that are tailored to specific experiments' needs. The Osaka/SPring-8 team has demonstrated that an adaptive mirror can be used to correct aberrations of focusing graded multilayer optics to obtain a sub-10-nm focal spot. The team also demonstrated that deformable mirror technology is suitable for building K-B zoom optics to provide coherent x-rays with controllable beam size for applications such as coherent diffraction imaging and microscopy.

9.2 Strategic plan

While the APS Optics Group does not have in-house expertise in producing adaptive x-ray mirror systems, it is exploring collaborations with other institutions and industry to test and make available adaptive optics for specific future needs at the APS.

10. Optical and at-wavelength metrology

10.1 Status

From the beginning of its operations, APS has had a metrology laboratory that houses an array of commercial and custom-made metrology instruments to measure mirrors, both to verify that the manufacturers have reached contract specifications in terms of surface roughness, slope, and shape errors, and to predict the performance of beamlines as built. The metrology lab includes a stitching interferometer for measurements of figure over sub-0.01mm- to 100-mm-length lateral scales, a laser Fizeau interferometer for surface figure measurement of optics up 150 mm in diameter at normal incidence angle, and a new long trace profilometer (LTP) that offers sub-50-nrad slope measurement accuracy on mirrors up to 1.5 m long. While the LTP is quite new, other metrology instruments are in need of replacement.

At-wavelength testing of optics is carried out at beamline 1-BM. A portable grating interferometer has been built for beam coherence and wavefront measurements. The system was commissioned during early FY 2016. It will be primarily used at 1-BM, but could be deployed at other APS beamlines. As well, rocking curve topography leading to high-resolution strain mapping has been implemented at 1-BM for the characterization of high-quality single crystals, especially diamonds, intended for use as x-ray optical elements.

Currently, beamline 1-BM contains five beryllium windows, each 0.25 mm thick, which severely affect the interpretation of coherence as well as high-resolution topography measurement data. Replacement of the double window in the 1-BM-A experiment hutch with a differential pumping setup, as done at beamlines 12-BM and 20-BM, is under way and should be completed in 2016. The remaining three windows cannot be replaced with differential pumping because they need to open onto experiment space in the 1-BM-B and 1-BM-C hutches.

10.2 Strategic plan

Future plans beyond 2016 include the following:

- Improving optical metrology tools by upgrading obsolete tools and developing new sensors.
- Developing in situ metrology and new coherence measurement techniques
- Improving the remaining three windows in beamline 1-BM by polishing, or possibly replacing them with diamond windows.
- Using an insertion device beamline for testing optics for the APS-U that require an x-ray beam with a smaller horizontal emittance, larger coherent flux, or larger power load than the beam that can be obtained from 1-BM.